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**Uniqueness results for
transient dynamics of quantum systems**

by

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Uniqueness Results for Transient Dynamics of Quantum Systems

Arne Jensen and Gheorghe Nenciu

Dedicated to Jean-Michel Combes on the occasion of his 65th birthday

ABSTRACT. Let H be a self-adjoint operator on a Hilbert space \mathcal{H} with an eigenvalue E_0 embedded either in the continuum or at a threshold. The eigenprojection P_0 is assumed to be of finite rank. Let W be a bounded self-adjoint operator. Let $H(\varepsilon) = H + \varepsilon W$ for ε small. If $P_0 e^{-itH(\varepsilon)} P_0 = e^{-ith(\varepsilon)} P_0 + \delta(\varepsilon, t)$ with $\sup_{t>0} \|\delta(\varepsilon, t)\| \leq C\varepsilon^p$ for some $p > 0$, then the effective Hamiltonian $h(\varepsilon)$ is uniquely determined up to a certain order in ε , which depends on the assumptions on $\text{Im } h(\varepsilon)$.

1. Introduction and results

In the papers [JN1, JN2, JN3] we have studied various aspects of perturbation of eigenvalues either embedded at a threshold, or embedded in the continuum proper. Let H be a self-adjoint operator on a Hilbert space \mathcal{H} . Assume that E_0 is an eigenvalue of H with eigenprojection P_0 , such that $0 < \text{Rank } P_0 < \infty$. Let W be a bounded self-adjoint operator, and consider the family $H(\varepsilon) = H + \varepsilon W$. Without loss of generality we can restrict to $0 \leq \varepsilon < \varepsilon_0$, with ε_0 sufficiently small.

In the papers mentioned we ask what happens to the eigenvalue E_0 for small ε . Under some assumptions we show that we get resonance behavior, in the form that we find an effective Hamiltonian $h(\varepsilon)$ on $P_0 \mathcal{H}$ and an error term $\delta(\varepsilon, t)$, such that

$$(1.1) \quad P_0 e^{-itH(\varepsilon)} P_0 = e^{-ith(\varepsilon)} P_0 + \delta(\varepsilon, t) \quad \text{for all } t > 0,$$

where

$$(1.2) \quad \sup_{t>0} \|\delta(\varepsilon, t)\| \leq C\varepsilon^p \quad \text{for some } p > 0.$$

We note that (1.1) and (1.2) together show that the resonance behavior will be observable for a finite time interval, provided ε is small enough.

The structure of the effective Hamiltonian $h(\varepsilon)$ depends on whether E_0 is an eigenvalue embedded in the continuum proper, or at a threshold. Furthermore, in

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the threshold case for $H = -\Delta + V$ on $L^2(\mathbf{R}^m)$, the structure depends on whether m is odd or even.

A natural question is to ask whether the effective Hamiltonian $h(\varepsilon)$ is unique. If $h(\varepsilon)$ has an asymptotic expansion as $\varepsilon \rightarrow 0$, the question is how many expansion coefficients are uniquely determined. The first result we are aware of is [CGH, Proposition 1.3]. These authors consider a simple embedded eigenvalue and obtain uniqueness for asymptotic expansion coefficients up to order ε^3 . The first result we state concerns also the rank one case. It is similar to the result [CGH, Proposition 1.3], but we state it in general, and give a somewhat simpler and different proof.

PROPOSITION 1.1. *Assume $\text{Rank } P_0 = 1$. Assume that $h^1(\varepsilon)$ and $h^2(\varepsilon)$ both satisfy (1.1) and (1.2), with the same value for p . Assume that for some $c_0 > 0$ and $q > 0$ we have*

$$(1.3) \quad -c_0 \varepsilon^q P_0 \leq \text{Im } h^1(\varepsilon) \leq 0 \quad \text{for } 0 \leq \varepsilon < \varepsilon_0.$$

Then for ε_0 sufficiently small we have

$$(1.4) \quad \|h^1(\varepsilon) - h^2(\varepsilon)\|_{\mathcal{B}(P_0\mathcal{H})} \leq C\varepsilon^{p+q}, \quad 0 \leq \varepsilon < \varepsilon_0.$$

One can easily write down an example showing that the result in Proposition 1.1 is optimal: The power of ε in (1.4) cannot be increased.

The second result is our main result and applies to the general case $1 \leq \text{Rank } P_0 < \infty$.

THEOREM 1.2. *Assume $1 \leq \text{Rank } P_0 < \infty$.*

(i) *Assume that $h^1(\varepsilon)$ and $h^2(\varepsilon)$ both satisfy (1.1) and (1.2), with the same value for p . Assume that $h^1(\varepsilon)$ satisfies*

$$(1.5) \quad h^1(\varepsilon) = E_0 P_0 + \varepsilon h_1^1 + \varepsilon f^1(\varepsilon), \quad 0 \leq \varepsilon < \varepsilon_0,$$

such that $h_1^1 = (h_1^1)^$, $\text{Im } f^1(\varepsilon) \leq 0$, and $f^1(\varepsilon) = o(1)$ as $\varepsilon \rightarrow 0$. Assume that $h^2(\varepsilon)$ is a bounded family of operators on $P_0\mathcal{H}$. Then for ε_0 sufficiently small we have*

$$(1.6) \quad \|h^1(\varepsilon) - h^2(\varepsilon)\|_{\mathcal{B}(P_0\mathcal{H})} \leq C\varepsilon^{p+1}, \quad 0 \leq \varepsilon < \varepsilon_0.$$

(ii) *Assume that $h^1(\varepsilon)$ and $h^2(\varepsilon)$ both satisfy (1.1) and (1.2), with $p = 2$. Assume that $h^1(\varepsilon)$ satisfies*

$$(1.7) \quad h^1(\varepsilon) = E_0 P_0 + \varepsilon h_1 + \varepsilon^2 h_2 + o(\varepsilon^2), \quad 0 \leq \varepsilon < \varepsilon_0,$$

such that $h_1 = h_1^$ and $\text{Im } h^1(\varepsilon) \leq 0$. Assume that $h^2(\varepsilon)$ is a bounded family of operators on $P_0\mathcal{H}$. Then there exists a family of invertible operators $U(\varepsilon)$ on $P_0\mathcal{H}$ with $U(\varepsilon) = P_0 + O(\varepsilon^2)$, such that for ε_0 sufficiently small we have*

$$(1.8) \quad \|h^1(\varepsilon) - U(\varepsilon)^{-1} h^2(\varepsilon) U(\varepsilon)\|_{\mathcal{B}(P_0\mathcal{H})} \leq C\varepsilon^4, \quad 0 \leq \varepsilon < \varepsilon_0.$$

A few remarks are in order here. As in the non-degenerate case one can give an example showing that the result in Theorem 1.2(i) is optimal (see Section 5 for details). As it stands, the uniqueness result in Theorem 1.2(i) is weaker than the result for the non-degenerate case. For example, take $p = 2$ and suppose $\text{Im } h^1(\varepsilon) \sim \varepsilon^2$. Then $p + q = 4$, while the error in 1.6 is of order ε^3 . The point is that (as the example in Section 5 shows) (1.1) and (1.2) put stronger constraints on the spectra of $h^j(\varepsilon)$ than on the operators themselves. This explains the result in Theorem 1.2(ii), as the spectra are invariant under the similarity transformations. At the level of spectra the results in Proposition 1.1 and Theorem 1.2(ii) agree, and as already said, are optimal.

The result in Theorem 1.2(ii) can be generalized. If we know that the coefficient h_2 in (1.7) is self-adjoint, i.e. $\operatorname{Im} h^1(\varepsilon) \sim \varepsilon^3$ at most, then the decomposition procedure in the proof of Theorem 1.2(ii) can be performed once more, leading to an estimate of the difference of order ε^5 . As long as the expansion coefficients are self-adjoint, the procedure can be iterated. We omit a formal statement of these results.

An important consequence of our results is that they make it possible to take (1.1) and (1.2) as the starting point for the *definition* of a resonance. In this context we refer to [H] for a review of various definitions of a resonance.

For papers with results of the form (1.1) and (1.2) we refer to the references and the comments in our papers [JN1, JN2, JN3]. We supplement this information by mentioning the paper [D], where error estimates are obtained for a one-dimensional Friedrichs' model.

2. Preliminaries

We recall some well-known general results that we need in the sequel. Let A and B be bounded operators on a Hilbert space \mathcal{H} . Then we have the estimates

$$(2.1) \quad \|e^A\| \leq e^{\|A\|}$$

and

$$(2.2) \quad \|e^A - I\| \leq \|A\|e^{\|A\|}.$$

We have

$$(2.3) \quad e^{-A} - e^{-B} = \int_0^1 e^{-(1-\tau)B}(B-A)e^{-\tau A}d\tau,$$

which implies the estimate

$$(2.4) \quad \|e^{-A} - e^{-B}\| \leq e^{\|A\|+\|B\|}\|A-B\|.$$

Assume that T is an $N \times N$ matrix satisfying $\operatorname{Im} T \leq 0$. Then it follows from the classical Lie product formula that

$$(2.5) \quad \|e^{-itT}\| \leq 1 \quad \text{for all } t \geq 0.$$

3. Proof, rank one case

We now give the proof of Proposition 1.1. We simplify the notation by writing $h^1(\varepsilon) = \lambda^1(\varepsilon)P_0$ and $h^2(\varepsilon) = \lambda^2(\varepsilon)P_0$. Thus we have

$$\sup_{t>0} \left| e^{-it\lambda^1(\varepsilon)} - e^{-it\lambda^2(\varepsilon)} \right| \leq C\varepsilon^p, \quad 0 \leq \varepsilon \leq \varepsilon_0.$$

Using the assumption on $\operatorname{Im} h^1(\varepsilon)$ we get

$$\left| 1 - e^{-it(\lambda^2(\varepsilon) - \lambda^1(\varepsilon))} \right| \leq C\varepsilon^p e^{tc_0\varepsilon^q}.$$

Thus by taking ε_0 sufficiently small, we can get

$$\left| 1 - e^{-it(\lambda^2(\varepsilon) - \lambda^1(\varepsilon))} \right| \leq \frac{1}{2}$$

for $0 \leq \varepsilon \leq \varepsilon_0$ and $0 < t \leq (c_0\varepsilon^q)^{-1}$. The above estimate implies that we can use the principal branch of the natural logarithm for these values of ε and t . An elementary estimate shows that

$$|\log(1-z) + z| \leq |z|^2, \quad |z| \leq \frac{1}{2}.$$

Thus we estimate as follows.

$$\begin{aligned} |-it(\lambda^2(\varepsilon) - \lambda^1(\varepsilon))| &= |\log(1 - (1 - e^{-it(\lambda^2(\varepsilon) - \lambda^1(\varepsilon))}))| \\ &\leq \frac{3}{2}|1 - e^{-it(\lambda^2(\varepsilon) - \lambda^1(\varepsilon))}| \leq C\varepsilon^p e^{tc_0\varepsilon^q}. \end{aligned}$$

Using this estimate for $t = \frac{1}{c_0\varepsilon^q}$ gives the result in Proposition 1.1.

4. Proof, general case

In the proof we can assume $E_0 = 0$, to simplify the arguments, since the operator $-itE_0P_0$ commutes with other operators in our computations below. We recall that for bounded operators on a Hilbert space we have the Dunford calculus. In our case we choose a domain in the complex plane as follows:

$$(4.1) \quad \mathcal{A} = \{re^{i\theta} \mid |r - 1| < \delta_0, |\theta| < \pi - 2\theta_0\}.$$

Here $\delta_0 > 0$ and $\theta_0 > 0$ are chosen sufficiently small. We let Γ denote a smooth positively oriented simple contour encircling the domain \mathcal{A} once, and contained in the domain

$$\{re^{i\theta} \mid \delta_0 < |r - 1| < 2\delta_0, |\theta| < \pi - \theta_0\}.$$

Let $\log z$ denote the principal branch of the natural logarithm, determined by $-\pi < \arg z \leq \pi$. Then for $z_0 \in \mathcal{A}$ we have

$$(4.2) \quad \log z_0 = \frac{-1}{2\pi i} \int_{\Gamma} (z_0 - z)^{-1} \log z \, dz.$$

In the Dunford calculus one replaces the z_0 on the right hand side by an operator A , in order to define $\log A$. To do this one must ensure that $\sigma(A) \subseteq \mathcal{A}$.

The assumptions in Theorem 1.2(i) imply that we have

$$(4.3) \quad \sup_{t>0} \|e^{-ith^1(\varepsilon)} - e^{-ith^2(\varepsilon)}\| \leq C\varepsilon^p, \quad 0 \leq \varepsilon < \varepsilon_0.$$

We now fix ε satisfying $0 < \varepsilon < \varepsilon_0$. During the proof we may choose a smaller value for ε_0 , but we keep the notation ε_0 . We will use the uniformity in t in (4.3) to take t depending on ε . We now fix $t = 1/\varepsilon$. We can assume that $\sigma(h_1^1) \subset (-\pi + 3\theta_0, \pi - 3\theta_0)$. Otherwise, we choose $c > 0$, such that this condition holds for ch_1^1 , and take $t = c/\varepsilon$. Using (2.3) we get

$$(4.4) \quad e^{-i(h_1^1 + f^1(\varepsilon))} - e^{-ih_1^1} = i \int_0^1 e^{-i(1-\tau)(h_1^1 + f^1(\varepsilon))} f^1(\varepsilon) e^{-i\tau h_1^1} d\tau.$$

Since $\text{Im}(h_1^1 + f^1(\varepsilon)) \leq 0$, we have from (2.5) that

$$\|e^{-i(1-\tau)(h_1^1 + f^1(\varepsilon))}\| \leq 1 \quad \text{for } 0 \leq \varepsilon < \varepsilon_0.$$

Since h_1^1 is assumed to be self-adjoint, we can use the spectral theorem to get a lower bound

$$\|e^{-ih_1^1} - z\| \geq C_2, \quad \text{for all } z \in \Gamma.$$

Using (4.4) and these estimates, and taking ε_0 smaller, if necessary, we get

$$(4.5) \quad \|(e^{-i(h_1^1 + f^1(\varepsilon))} - z)^{-1}\| \leq C_3, \quad z \in \Gamma, \quad 0 \leq \varepsilon < \varepsilon_0.$$

Next we use the second resolvent equation and (4.3) to get

$$(4.6) \quad \|(e^{-i\frac{1}{\varepsilon}h^2(\varepsilon)} - z)^{-1}\| \leq C_3, \quad z \in \Gamma, \quad 0 \leq \varepsilon < \varepsilon_0.$$

The spectrum of $e^{-i\frac{1}{\varepsilon}h^1(\varepsilon)}$ lies in \mathcal{A} , at least for ε_0 sufficiently small. The same holds for the spectrum of $e^{-i\frac{1}{\varepsilon}h^2(\varepsilon)}$, due to (4.3) and elementary perturbation theory, again if ε_0 is sufficiently small. Thus we can apply the Dunford calculus to get

$$(4.7) \quad h^1(\varepsilon) - h^2(\varepsilon) = \frac{\varepsilon}{2\pi} \int_{\Gamma} (\log z) (e^{-i\frac{1}{\varepsilon}h^1(\varepsilon)} - z)^{-1} \\ \times [e^{-i\frac{1}{\varepsilon}h^1(\varepsilon)} - e^{-i\frac{1}{\varepsilon}h^2(\varepsilon)}] (e^{-i\frac{1}{\varepsilon}h^2(\varepsilon)} - z)^{-1} dz.$$

Using (4.3), (4.5), and (4.6), we get

$$(4.8) \quad \|h^1(\varepsilon) - h^2(\varepsilon)\| \leq C\varepsilon^{1+p}, \quad 0 \leq \varepsilon < \varepsilon_0.$$

Thus the result in Theorem 1.2(i) is proved.

Proof of Theorem 1.2(ii). First we apply Theorem 1.2(i) to conclude that

$$(4.9) \quad \|h^1(\varepsilon) - h^2(\varepsilon)\| \leq C\varepsilon^3,$$

and thus

$$h^2(\varepsilon) = E_0 P_0 + \varepsilon h_1 + \varepsilon^2 h_2 + o(\varepsilon^2).$$

Now we divide the proof into two cases. Consider first the case $h_1 = \mu P_0$ for some real μ . Then $E_0 P_0 + \varepsilon h_1$ commutes with all other operators. Now due to the assumptions the estimate (4.3) holds with $p = 2$. We can factor out $e^{-it(E_0 P_0 + \varepsilon h_1)}$. Define

$$\hat{h}^j(\varepsilon) = \frac{1}{\varepsilon^2} (h^j(\varepsilon) - E_0 P_0 - \varepsilon h_1), \quad j = 1, 2.$$

Taking $s = t\varepsilon^2$ it follows that we have the estimate

$$\sup_{s>0} \|e^{-is\hat{h}^1(\varepsilon)} - e^{-is\hat{h}^2(\varepsilon)}\| \leq C, \quad 0 \leq \varepsilon < \varepsilon_0.$$

Now since h_2 is not known to be self-adjoint (and usually is not self-adjoint), we need an argument different from the one used in the proof of Theorem 1.2(i).

We use the estimate (2.2) for a sufficiently small s_0 to get

$$\|e^{-is_0\hat{h}^j(\varepsilon)} - P_0\| \leq \frac{1}{4}, \quad 0 \leq \varepsilon < \varepsilon_0, \quad j = 1, 2.$$

This estimate implies that the numerical range of $e^{-is_0\hat{h}^j(\varepsilon)}$ is contained in the set $\{z \mid |z - 1| < \frac{1}{4}\}$. Take as a contour the circle $\Gamma_1 = \{z \mid |z - 1| = \frac{1}{2}\}$. Now we use the resolvent estimate related to the numerical range, see [K, Theorem V.3.2], to get

$$\|(e^{-is_0\hat{h}^j(\varepsilon)} - z)^{-1}\| \leq C, \quad z \in \Gamma_1, \quad 0 \leq \varepsilon < \varepsilon_0, \quad j = 1, 2.$$

We can then use the Dunford calculus for the logarithm, with the contour Γ_1 , as in the proof of Theorem 1.2(i), to get

$$\|\hat{h}^1(\varepsilon) - \hat{h}^2(\varepsilon)\| \leq C\varepsilon^2.$$

Note that we have a fixed s_0 , so we do not gain an extra factor ε , as in (4.7). Thus in the $h_1 = \mu P_0$ case we have proved that

$$\|h^1(\varepsilon) - h^2(\varepsilon)\| \leq C\varepsilon^4.$$

Now we consider the case where $h_1 \neq \mu P_0$. Since h_1 is assumed self-adjoint, it must have at least two distinct real eigenvalues. We denote the distinct eigenvalues of h_1 by

$$\lambda_1, \lambda_2, \dots, \lambda_m, \quad m \leq \text{Rank } P_0.$$

We now recall some basic facts from eigenvalue perturbation theory. All results needed can be found in [K]. We introduce the operators

$$(4.10) \quad \tilde{h}^j(\varepsilon) = \frac{1}{\varepsilon}(h^j(\varepsilon) - E_0 P_0), \quad j = 1, 2.$$

Both operators have the self-adjoint operator h_1 as their leading term. Each eigenvalue λ_q of h_1 gives rise to a group of eigenvalues of $\tilde{h}^j(\varepsilon)$, $j = 1, 2$. The Riesz projection for this eigenvalue group is denoted by $P_q^j(\varepsilon)$. These projections have the following properties:

$$(4.11) \quad P_q^j(\varepsilon)P_{q'}^j(\varepsilon) = \delta_{q,q'}P_q^j(\varepsilon), \quad \sum_{q=1}^m P_q^j(\varepsilon) = P_0,$$

for $j = 1, 2$, $q, q' = 1, 2, \dots, m$, and for all $0 \leq \varepsilon < \varepsilon_0$.

The estimate (4.9) implies $\|\tilde{h}^1(\varepsilon) - \tilde{h}^2(\varepsilon)\| \leq C\varepsilon^2$. Since the $P_q^j(\varepsilon)$ are the Riesz projections, it follows that

$$\|P_q^1(\varepsilon) - P_q^2(\varepsilon)\| \leq C\varepsilon^2, \quad q = 1, 2, \dots, m.$$

Define the (not normalized) Sz.-Nagy operator

$$U(\varepsilon) = \sum_{q=1}^m P_q^2(\varepsilon)P_q^1(\varepsilon).$$

The results in (4.11) imply that

$$U(\varepsilon) - P_0 = \sum_{q=1}^m (P_q^2(\varepsilon) - P_q^1(\varepsilon))P_q^1(\varepsilon),$$

such that

$$\|U(\varepsilon) - P_0\| \leq C\varepsilon^2.$$

Thus $U(\varepsilon)$ is invertible in $P_0\mathcal{H}$ for all $0 \leq \varepsilon < \varepsilon_0$, if ε_0 is sufficiently small. It follows from the Neumann series that

$$\|U(\varepsilon)^{-1} - P_0\| \leq C\varepsilon^2.$$

The definition implies that $U(\varepsilon)P_q^1(\varepsilon) = P_q^2(\varepsilon)U(\varepsilon)$, such that

$$P_q^2(\varepsilon) = U(\varepsilon)P_q^1(\varepsilon)U(\varepsilon)^{-1}, \quad q = 1, 2, \dots, m.$$

Define $k^2(\varepsilon) = U(\varepsilon)^{-1}\tilde{h}^2(\varepsilon)U(\varepsilon)$. Then we have

$$\|e^{-is\tilde{h}^2(\varepsilon)} - e^{-isk^2(\varepsilon)}\| = \|e^{-is\tilde{h}^2(\varepsilon)} - U(\varepsilon)^{-1}e^{-is\tilde{h}^2(\varepsilon)}U(\varepsilon)\| \leq C_s\varepsilon^2.$$

Note that the constant may depend on s . This does not cause problems, since the estimate is used only for a fixed value of s . It follows that we have

$$(4.12) \quad \|e^{-is\tilde{h}^1(\varepsilon)} - e^{-isk^2(\varepsilon)}\| \leq C_s\varepsilon^2.$$

Due to the definition of $U(\varepsilon)$ we have $[P_q^1(\varepsilon), k^2(\varepsilon)] = 0$, $q = 1, 2, \dots, m$. Thus we can find families of operators $\tilde{h}_q^1(\varepsilon)$ and $k_q^2(\varepsilon)$ on $P_q^1(\varepsilon)\mathcal{H}$, such that

$$\tilde{h}^1(\varepsilon) = \sum_{q=1}^m \tilde{h}_q^1(\varepsilon)P_q^1(\varepsilon) \quad \text{and} \quad k^2(\varepsilon) = \sum_{q=1}^m k_q^2(\varepsilon)P_q^1(\varepsilon).$$

We have that

$$\tilde{h}_q^1(\varepsilon) = \lambda_q P_q^1(0) + O(\varepsilon) \quad \text{and} \quad k_q^2(\varepsilon) = \lambda_q P_q^1(0) + O(\varepsilon).$$

Furthermore, we have

$$e^{-is\tilde{h}^1(\varepsilon)} = \sum_{q=1}^m e^{-is\tilde{h}_q^1(\varepsilon)} P_q^1(\varepsilon) \quad \text{and} \quad e^{-isk^2(\varepsilon)} = \sum_{q=1}^m e^{-isk_q^2(\varepsilon)} P_q^1(\varepsilon).$$

It follows from (4.12) that on $P_q^1(0)\mathcal{H}$ we have

$$\|e^{-is\tilde{h}_q^1(\varepsilon)} - e^{-isk_q^2(\varepsilon)}\| \leq C\varepsilon^2.$$

Thus we can repeat the argument from the first case, i.e. $h_1 = \mu P_0$, in the space $P_q^1(0)\mathcal{H}$. Putting the pieces together yields the estimate (1.8).

5. An example

We give an example showing that the result in Theorem 1.2(i) is optimal in the case $\text{Rank } P_0 \geq 2$. We consider operators on $P_0\mathcal{H}$, assuming $2 \leq \text{Rank } P_0 < \infty$. We will assume $E_0 = 0$. Take an operator

$$h^1(\varepsilon) = \varepsilon h_1^1 + o(\varepsilon), \quad \text{Im } h^1(\varepsilon) \leq 0,$$

and a family of unitary operators $W(\varepsilon)$, such that $\varepsilon \mapsto W(\varepsilon)$ is at least continuously differentiable, and $W(0) = P_0$. Define

$$h^2(\varepsilon) = W(\varepsilon)^* h^1(\varepsilon) W(\varepsilon).$$

Thus we know that $\sigma(h^1(\varepsilon)) = \sigma(h^2(\varepsilon))$ for all ε . For $0 \leq \varepsilon < \varepsilon_0$ with ε_0 sufficiently small we can define $S(\varepsilon) = \log W(\varepsilon)$, where we take the principal branch of the logarithm. $S(\varepsilon)$ is a normal operator, so we have

$$W(\varepsilon)^* W(\varepsilon) = e^{S(\varepsilon)^* + S(\varepsilon)} = P_0,$$

which implies that $S(\varepsilon) = iT(\varepsilon)$ for some self-adjoint operator $T(\varepsilon)$. Furthermore, $T(\varepsilon) = \varepsilon T_1 + o(\varepsilon)$. Now we have

$$\begin{aligned} h^1(\varepsilon) - h^2(\varepsilon) &= W(\varepsilon)^* (W(\varepsilon) h^1(\varepsilon) - h^1(\varepsilon) W(\varepsilon)) \\ &= W(\varepsilon)^* [W(\varepsilon) - P_0, h^1(\varepsilon)], \end{aligned}$$

which implies

$$(5.1) \quad \|h^1(\varepsilon) - h^2(\varepsilon)\| \leq C\varepsilon^2.$$

In the same manner we get

$$(5.2) \quad e^{-ith^1(\varepsilon)} - e^{-ith^2(\varepsilon)} = W(\varepsilon)^* [W(\varepsilon) - P_0, e^{-ith^1(\varepsilon)}].$$

It follows that

$$(5.3) \quad \sup_{t>0} \|e^{-ith^1(\varepsilon)} - e^{-ith^2(\varepsilon)}\| \leq C\varepsilon.$$

We now verify that for some choices of $W(\varepsilon)$ the estimates (5.1) and (5.3) cannot be improved. Consider first (5.1). We have

$$\lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon^2} (h^1(\varepsilon) - h^2(\varepsilon)) = \lim_{\varepsilon \downarrow 0} W(\varepsilon)^* \left[\frac{1}{\varepsilon} (W(\varepsilon) - P_0), h_1^1 + o(1) \right] = i[T_1, h_1^1].$$

In dimensions greater than one it is always possible to find T_1 and h_1^1 , such that this commutator is nonzero.

In the case of (5.3) the crucial point is the uniformity in t . We take $t = 1/\varepsilon$ and then compute as above to find

$$\lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon} (e^{-i\frac{1}{\varepsilon}h^1(\varepsilon)} - e^{-i\frac{1}{\varepsilon}h^2(\varepsilon)}) = i[T_1, e^{-ih_1^1}].$$

By a suitable choice of T_1 and h_1^1 both commutators can be made nonzero.

These results show that Theorem 1.2(i) in general is optimal.

6. Applications

We will briefly state some consequences of Proposition 1.1 and Theorem 1.2 for the results obtained in [JN1, JN3]. Consider first the case $\text{Rank } P_0 = 1$. For a simple eigenvalue embedded at a threshold we obtained in [JN1, Theorem 3.7] an effective Hamiltonian of the form $h(\varepsilon) = \lambda(\varepsilon)P_0$, with the following structure:

$$(6.1) \quad \begin{aligned} \lambda(\varepsilon) &= x_0(\varepsilon) - i\Gamma(\varepsilon), \\ x_0(\varepsilon) &= b\varepsilon(1 + \mathcal{O}(\varepsilon)), \end{aligned}$$

$$(6.2) \quad \Gamma(\varepsilon) = \gamma_\nu \varepsilon^{2+(\nu/2)}(1 + \mathcal{O}(\varepsilon)).$$

Here b and γ_ν are positive constants, and ν is an odd integer, $\nu = -1, 1, \dots$. The result (1.1) is proved with an error term (1.2) with $p = p(\nu) = \min\{2, (2 + \nu)/2\}$. This gives the following results for the constant $p + q$ in (1.4). For $\nu = -1$ it equals 2, for $\nu = 1$ it equals 4, and for $\nu \geq 3$ it equals $4 + (\nu/2)$. Thus the terms in $h(\varepsilon)$ are unique up to that order. As shown by (6.1) and (6.2), we have obtained the leading terms explicitly. We should mention that in the papers cited above explicit examples for all admissible values of ν are given.

To state some results for the case of an eigenvalue embedded in the continuum proper, we need to recall some definitions. For $a > 0$ we define

$$(6.3) \quad D_a(E_0) = \{z \in \mathbf{C} \mid |z - E_0| < a, \text{Im } z > 0\}.$$

We denote by $C^{n,\theta}(D_a(E_0))$ the functions in $D_a(E_0)$ that are n times continuously norm-differentiable, with the n^{th} derivative satisfying a uniform Hölder condition in $D_a(E_0)$, of order θ , $0 \leq \theta \leq 1$. The derivatives are also assumed uniformly bounded in $D_a(E_0)$. As above we assume that H is a self-adjoint operator on \mathcal{H} , such that E_0 is an eigenvalue of H of finite multiplicity embedded in the continuum. Again, the eigenprojection is denoted by P_0 . We also need $Q_0 = I - P_0$. We assume that W is a bounded operator on \mathcal{H} , which is factored as

$$(6.4) \quad W = A^*DA,$$

where $D^* = D$ and $D^2 = I$. We introduce the operator family

$$(6.5) \quad G(z) = AQ_0(H - z)^{-1}Q_0A^*.$$

One of the results in [JN3] can then be stated as follows.

THEOREM 6.1. [JN3, Theorem 4] *Assume $2 \leq \text{Rank } P_0 < \infty$. Assume that $G(z) \in C^{n,\theta}(D_a(E_0))$ with $n + \theta \geq 2$. Assume*

$$(6.6) \quad \text{Im } P_0A^*DG(E_0 + i0)DAP_0 > 0 \quad \text{on } P_0\mathcal{H}.$$

Then there exists a function $\delta(\varepsilon, t)$ satisfying (1.2) with $p = 2$, such that

$$(6.7) \quad P_0e^{-itH(\varepsilon)}P_0 = e^{-it h(\varepsilon)}P_0 + \delta(\varepsilon, t).$$

Here $h(\varepsilon)$ on $P_0\mathcal{H}$ is given by

$$(6.8) \quad h(\varepsilon) = E_0 P_0 + \varepsilon P_0 W P_0 - \varepsilon^2 P_0 W Q_0 (H - E_0 - i0)^{-1} Q_0 W P_0 \\ - \varepsilon^3 \left\{ P_0 W Q_0 (H - E_0 - i0)^{-1} Q_0 W Q_0 (H - E_0 - i0)^{-1} Q_0 W P_0 \right. \\ \left. + \frac{1}{2} \left[P_0 W P_0 W \frac{d}{dE} Q_0 (H - E - i0)^{-1} Q_0 \Big|_{E=E_0} W P_0 \right. \right. \\ \left. \left. + P_0 W \frac{d}{dE} Q_0 (H - E - i0)^{-1} Q_0 \Big|_{E=E_0} W P_0 W P_0 \right] \right\}.$$

Comparing with the statement in [JN3] we should note that the assumption (6.6) implies for some $\gamma > 0$ that we have

$$(6.9) \quad \operatorname{Im} P_0 A^* D G(E_0 + i0) D A P_0 \geq \gamma P_0,$$

since $P_0\mathcal{H}$ is finite dimensional.

Our Theorem 1.2(i) can be applied to this result, and leads to the conclusion that the terms up to order 2 given in (6.8) are uniquely determined. Moreover by Theorem 1.2(ii), up to a similarity transformation, the coefficients given in (6.8) are unique up to the order ε^3 .

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References

- [CGH] L. Cattaneo, G.M. Graf, and W. Hunziker, *A general resonance theory based on Mourre's inequality*, Ann. H. Poincaré **7** (2006), 583–614.
- [D] M. Demuth, *Pole approximation and spectral concentration*, Math. Nachr. **73** (1976), 65–72.
- [H] E. M. Harrell II, *Perturbation theory and atomic resonances since Schrödinger's time*, preprint 2006.
- [JN1] A. Jensen and G. Nenciu, *The Fermi golden rule and its form at thresholds in odd dimensions*, Comm. Math. Phys. **261** (2006), 693–727.
- [JN2] A. Jensen and G. Nenciu, *Schrödinger operators on the half line: Resolvent expansions and the Fermi golden rule at thresholds*, Proc. Indian Acad. Sci. (Math. Sci.) **116** (2006), 375–392.
- [JN3] A. Jensen and G. Nenciu, *On the Fermi golden rule: Degenerate eigenvalues*, Proc. Conf. Operator Theory and Mathematical Physics, Bucharest, August 2005. To appear.
- [K] T. Kato, *Perturbation theory for linear operators*, Springer-Verlag, New York, 1966.

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